



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:28 AM UTC

PDB ID : 3T4W / pdb_00003t4w
Title : The crystal structure of mandelate racemase/muconate lactonizing enzyme from Sulfitobacter sp
Authors : Zhang, Z.; Chamala, S.; Evans, B.; Foti, R.; Gizzi, A.; Hillerich, B.; Kar, A.; LaFleur, J.; Seidel, R.; Villigas, G.; Zencheck, W.; Almo, S.C.; Swaminathan, S.; New York Structural Genomics Research Consortium (NYSGRG)
Deposited on : 2011-07-26
Resolution : 2.52 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

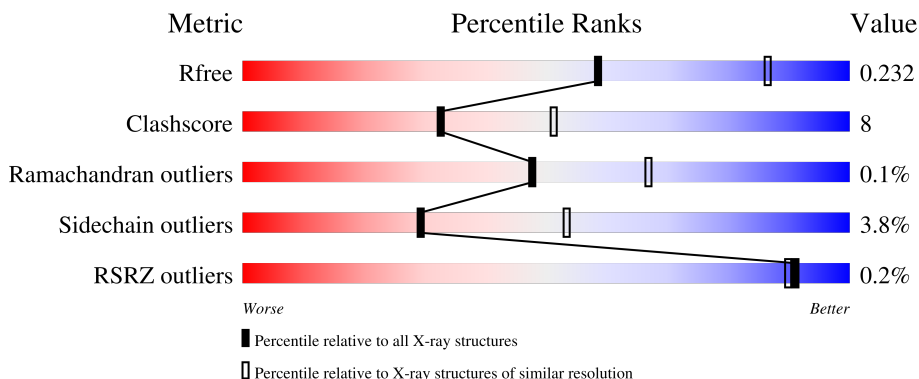
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	432	
1	B	432	
1	C	432	
1	D	432	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12495 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Mandelate racemase/muconate lactonizing enzyme family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3011	1922	514	553	22			
1	B	396	Total	C	N	O	S	0	0	0
			3011	1922	514	553	22			
1	C	396	Total	C	N	O	S	0	0	0
			3011	1922	514	553	22			
1	D	396	Total	C	N	O	S	0	0	0
			3011	1922	514	553	22			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP A3SSE3
A	-20	HIS	-	expression tag	UNP A3SSE3
A	-19	HIS	-	expression tag	UNP A3SSE3
A	-18	HIS	-	expression tag	UNP A3SSE3
A	-17	HIS	-	expression tag	UNP A3SSE3
A	-16	HIS	-	expression tag	UNP A3SSE3
A	-15	HIS	-	expression tag	UNP A3SSE3
A	-14	SER	-	expression tag	UNP A3SSE3
A	-13	SER	-	expression tag	UNP A3SSE3
A	-12	GLY	-	expression tag	UNP A3SSE3
A	-11	VAL	-	expression tag	UNP A3SSE3
A	-10	ASP	-	expression tag	UNP A3SSE3
A	-9	LEU	-	expression tag	UNP A3SSE3
A	-8	GLY	-	expression tag	UNP A3SSE3
A	-7	THR	-	expression tag	UNP A3SSE3
A	-6	GLU	-	expression tag	UNP A3SSE3
A	-5	ASN	-	expression tag	UNP A3SSE3
A	-4	LEU	-	expression tag	UNP A3SSE3
A	-3	TYR	-	expression tag	UNP A3SSE3
A	-2	PHE	-	expression tag	UNP A3SSE3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLN	-	expression tag	UNP A3SSE3
A	0	SER	-	expression tag	UNP A3SSE3
B	-21	MET	-	expression tag	UNP A3SSE3
B	-20	HIS	-	expression tag	UNP A3SSE3
B	-19	HIS	-	expression tag	UNP A3SSE3
B	-18	HIS	-	expression tag	UNP A3SSE3
B	-17	HIS	-	expression tag	UNP A3SSE3
B	-16	HIS	-	expression tag	UNP A3SSE3
B	-15	HIS	-	expression tag	UNP A3SSE3
B	-14	SER	-	expression tag	UNP A3SSE3
B	-13	SER	-	expression tag	UNP A3SSE3
B	-12	GLY	-	expression tag	UNP A3SSE3
B	-11	VAL	-	expression tag	UNP A3SSE3
B	-10	ASP	-	expression tag	UNP A3SSE3
B	-9	LEU	-	expression tag	UNP A3SSE3
B	-8	GLY	-	expression tag	UNP A3SSE3
B	-7	THR	-	expression tag	UNP A3SSE3
B	-6	GLU	-	expression tag	UNP A3SSE3
B	-5	ASN	-	expression tag	UNP A3SSE3
B	-4	LEU	-	expression tag	UNP A3SSE3
B	-3	TYR	-	expression tag	UNP A3SSE3
B	-2	PHE	-	expression tag	UNP A3SSE3
B	-1	GLN	-	expression tag	UNP A3SSE3
B	0	SER	-	expression tag	UNP A3SSE3
C	-21	MET	-	expression tag	UNP A3SSE3
C	-20	HIS	-	expression tag	UNP A3SSE3
C	-19	HIS	-	expression tag	UNP A3SSE3
C	-18	HIS	-	expression tag	UNP A3SSE3
C	-17	HIS	-	expression tag	UNP A3SSE3
C	-16	HIS	-	expression tag	UNP A3SSE3
C	-15	HIS	-	expression tag	UNP A3SSE3
C	-14	SER	-	expression tag	UNP A3SSE3
C	-13	SER	-	expression tag	UNP A3SSE3
C	-12	GLY	-	expression tag	UNP A3SSE3
C	-11	VAL	-	expression tag	UNP A3SSE3
C	-10	ASP	-	expression tag	UNP A3SSE3
C	-9	LEU	-	expression tag	UNP A3SSE3
C	-8	GLY	-	expression tag	UNP A3SSE3
C	-7	THR	-	expression tag	UNP A3SSE3
C	-6	GLU	-	expression tag	UNP A3SSE3
C	-5	ASN	-	expression tag	UNP A3SSE3
C	-4	LEU	-	expression tag	UNP A3SSE3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	TYR	-	expression tag	UNP A3SSE3
C	-2	PHE	-	expression tag	UNP A3SSE3
C	-1	GLN	-	expression tag	UNP A3SSE3
C	0	SER	-	expression tag	UNP A3SSE3
D	-21	MET	-	expression tag	UNP A3SSE3
D	-20	HIS	-	expression tag	UNP A3SSE3
D	-19	HIS	-	expression tag	UNP A3SSE3
D	-18	HIS	-	expression tag	UNP A3SSE3
D	-17	HIS	-	expression tag	UNP A3SSE3
D	-16	HIS	-	expression tag	UNP A3SSE3
D	-15	HIS	-	expression tag	UNP A3SSE3
D	-14	SER	-	expression tag	UNP A3SSE3
D	-13	SER	-	expression tag	UNP A3SSE3
D	-12	GLY	-	expression tag	UNP A3SSE3
D	-11	VAL	-	expression tag	UNP A3SSE3
D	-10	ASP	-	expression tag	UNP A3SSE3
D	-9	LEU	-	expression tag	UNP A3SSE3
D	-8	GLY	-	expression tag	UNP A3SSE3
D	-7	THR	-	expression tag	UNP A3SSE3
D	-6	GLU	-	expression tag	UNP A3SSE3
D	-5	ASN	-	expression tag	UNP A3SSE3
D	-4	LEU	-	expression tag	UNP A3SSE3
D	-3	TYR	-	expression tag	UNP A3SSE3
D	-2	PHE	-	expression tag	UNP A3SSE3
D	-1	GLN	-	expression tag	UNP A3SSE3
D	0	SER	-	expression tag	UNP A3SSE3

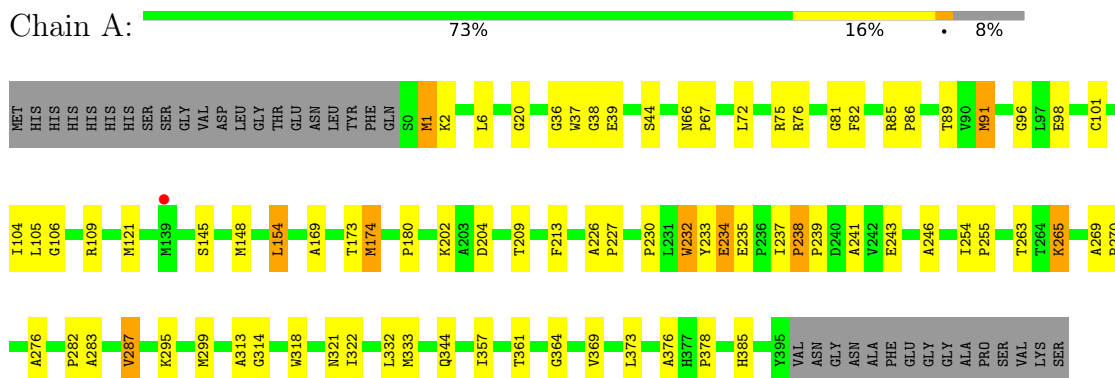
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	122	Total O 122 122	0	0
2	B	108	Total O 108 108	0	0
2	C	107	Total O 107 107	0	0
2	D	114	Total O 114 114	0	0

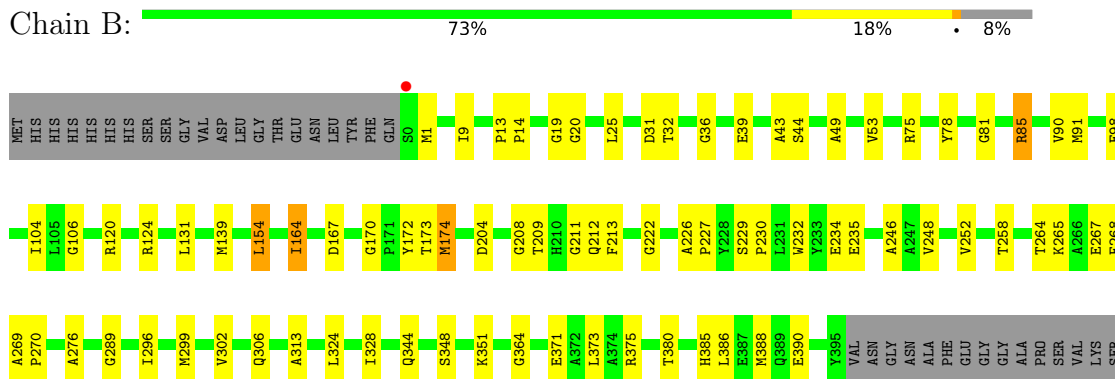
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

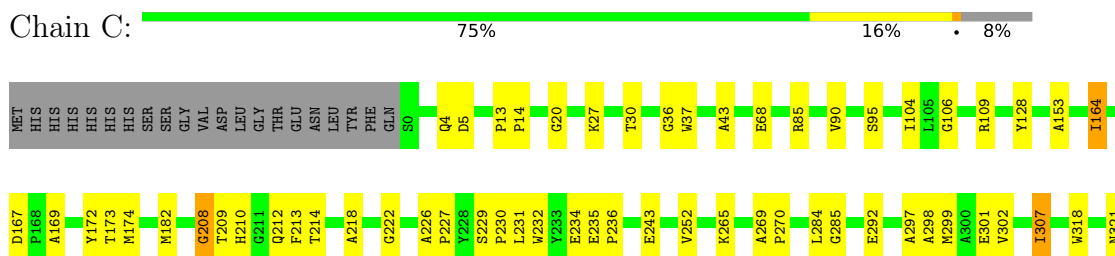
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme family protein

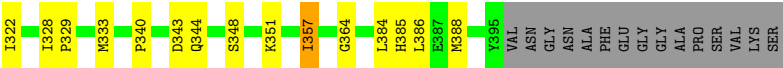


- Molecule 1: Mandelate racemase/muconate lactonizing enzyme family protein

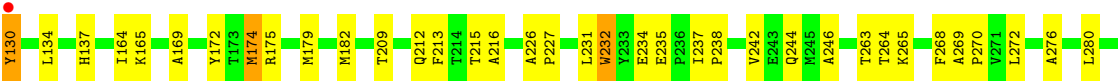


- Molecule 1: Mandelate racemase/muconate lactonizing enzyme family protein





● Molecule 1: Mandelate racemase/muconate lactonizing enzyme family protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	114.56Å 170.18Å 84.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.52 – 2.52 47.52 – 2.52	Depositor EDS
% Data completeness (in resolution range)	97.4 (47.52-2.52) 99.5 (47.52-2.52)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.48 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.184 , 0.240 0.180 , 0.232	Depositor DCC
R_{free} test set	2850 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.815	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 29.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12495	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.61	7/3092 (0.2%)	0.82	2/4218 (0.0%)
1	B	0.45	1/3092 (0.0%)	0.83	4/4218 (0.1%)
1	C	0.46	1/3092 (0.0%)	0.79	0/4218
1	D	0.45	0/3092	0.81	0/4218
All	All	0.50	9/12368 (0.1%)	0.81	6/16872 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	241	ALA	CA-CB	-7.60	1.44	1.53
1	A	232	TRP	C-O	-6.30	1.16	1.23
1	A	239	PRO	C-O	-5.95	1.17	1.23
1	A	234	GLU	C-O	-5.74	1.16	1.23
1	B	211	GLY	C-O	-5.36	1.16	1.24
1	A	2	LYS	C-O	-5.28	1.17	1.24
1	C	208	GLY	C-O	-5.28	1.16	1.23
1	A	233	TYR	C-O	-5.17	1.18	1.24
1	A	238	PRO	C-O	-5.12	1.18	1.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	314	GLY	CA-C-N	6.30	125.92	119.56
1	A	314	GLY	C-N-CA	6.30	125.92	119.56
1	B	328	ILE	N-CA-C	6.11	114.88	107.61
1	B	213	PHE	N-CA-C	5.39	118.52	109.95
1	B	170	GLY	CA-C-N	5.23	124.99	119.76
1	B	170	GLY	C-N-CA	5.23	124.99	119.76

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3011	0	2962	52	0
1	B	3011	0	2962	48	0
1	C	3011	0	2962	50	0
1	D	3011	0	2962	63	0
2	A	122	0	0	2	0
2	B	108	0	0	1	0
2	C	107	0	0	0	0
2	D	114	0	0	3	0
All	All	12495	0	11848	188	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (188) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:349:THR:HG21	1:D:367:LEU:HA	1.53	0.91
1:A:322:ILE:HD13	1:A:357:ILE:HG21	1.53	0.90
1:C:167:ASP:HB2	1:C:208:GLY:O	1.79	0.82
1:D:215:THR:OG1	1:D:244:GLN:HG3	1.80	0.80
1:C:322:ILE:HD13	1:C:357:ILE:HG21	1.63	0.80
1:A:20:GLY:HA3	1:A:385:HIS:CE1	2.18	0.78
1:A:322:ILE:CD1	1:A:357:ILE:HG21	2.16	0.76
1:A:332:LEU:HG	1:A:333:MET:HG2	1.68	0.75
1:B:90:VAL:HG21	1:D:44:SER:HB3	1.71	0.72
1:D:20:GLY:HA3	1:D:385:HIS:CE1	2.28	0.68
1:D:124:ARG:HD3	2:D:468:HOH:O	1.93	0.68
1:A:269:ALA:HB3	1:A:270:PRO:HD3	1.75	0.68
1:B:265:LYS:HB2	1:B:299:MET:HE1	1.75	0.68
1:D:269:ALA:HB3	1:D:270:PRO:HD3	1.75	0.67
1:A:1:MET:HE3	1:A:67:PRO:CG	2.26	0.66
1:A:91:MET:HA	1:A:91:MET:HE2	1.77	0.65
1:D:106:GLY:HA3	1:D:364:GLY:HA2	1.78	0.65
1:D:174:MET:HE2	1:D:175:ARG:HA	1.78	0.64
1:D:265:LYS:HB2	1:D:299:MET:HE1	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:MET:HE2	1:D:175:ARG:CA	2.28	0.63
1:B:386:LEU:O	1:D:81:GLY:HA2	1.98	0.62
1:A:106:GLY:HA3	1:A:364:GLY:HA2	1.82	0.61
1:D:174:MET:HE2	1:D:175:ARG:N	2.15	0.61
1:A:44:SER:HB3	1:C:90:VAL:HG21	1.83	0.60
1:C:172:TYR:HB3	1:C:212:GLN:HG3	1.84	0.59
1:C:269:ALA:HB3	1:C:270:PRO:HD3	1.83	0.59
1:B:78:TYR:HD1	1:B:91:MET:HE3	1.67	0.59
1:C:297:ALA:HA	1:C:307:ILE:HD11	1.85	0.59
1:B:269:ALA:HB3	1:B:270:PRO:HD3	1.85	0.58
1:D:169:ALA:HB1	1:D:213:PHE:HZ	1.69	0.58
1:D:1:MET:HE2	2:D:501:HOH:O	2.03	0.57
1:B:204:ASP:OD1	1:C:182:MET:HG2	2.05	0.57
1:D:105:LEU:O	1:D:109:ARG:HG2	2.05	0.57
1:A:1:MET:HE3	1:A:67:PRO:HG3	1.88	0.56
1:D:174:MET:HE2	1:D:174:MET:C	2.31	0.55
1:D:232:TRP:C	1:D:232:TRP:CD1	2.84	0.55
1:A:76:ARG:HG3	1:C:174:MET:HE3	1.88	0.54
1:B:174:MET:HE3	1:B:390:GLU:HA	1.88	0.54
1:D:72:LEU:HD21	1:D:76:ARG:NH2	2.21	0.54
1:D:174:MET:CE	1:D:175:ARG:HG3	2.38	0.54
1:A:237:ILE:HB	1:A:238:PRO:HD2	1.90	0.54
1:A:91:MET:HA	1:A:91:MET:CE	2.38	0.54
1:B:106:GLY:HA3	1:B:364:GLY:HA2	1.90	0.54
1:A:81:GLY:HA2	1:C:386:LEU:O	2.08	0.54
1:D:231:LEU:C	1:D:231:LEU:HD23	2.33	0.53
1:A:295:LYS:O	1:A:299:MET:HG3	2.08	0.53
1:B:131:LEU:HD11	1:B:164:ILE:HD13	1.88	0.53
1:C:322:ILE:CD1	1:C:357:ILE:HG21	2.36	0.53
1:D:376:ALA:C	1:D:378:PRO:HD3	2.34	0.53
1:D:246:ALA:HA	1:D:276:ALA:HA	1.91	0.53
1:B:44:SER:HB3	1:D:90:VAL:HG21	1.90	0.52
1:B:174:MET:HG2	1:D:75:ARG:HB3	1.90	0.52
1:A:283:ALA:O	1:A:287:VAL:HG22	2.09	0.52
1:B:306:GLN:HG3	1:C:214:THR:HG21	1.90	0.52
1:A:344:GLN:HG3	1:A:373:LEU:HD21	1.92	0.51
1:A:322:ILE:HD13	1:A:357:ILE:CG2	2.35	0.51
1:A:1:MET:HE3	1:A:67:PRO:HG2	1.92	0.51
1:C:43:ALA:O	1:C:384:LEU:HD13	2.11	0.51
1:C:68:GLU:HG2	1:C:109:ARG:HH22	1.75	0.51
1:A:145:SER:OG	1:A:148:MET:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:348:SER:HB3	1:C:351:LYS:HE3	1.93	0.51
1:D:318:TRP:O	1:D:321:ASN:HB2	2.12	0.50
1:A:376:ALA:C	1:A:378:PRO:HD3	2.36	0.50
1:C:265:LYS:HG2	1:C:292:GLU:OE2	2.11	0.50
1:D:39:GLU:OE2	1:D:313:ALA:HB1	2.11	0.50
1:C:153:ALA:HB1	1:C:164:ILE:HD12	1.93	0.50
1:D:347:LYS:HD2	1:D:368:GLU:HG2	1.92	0.50
1:A:318:TRP:O	1:A:321:ASN:HB2	2.11	0.50
1:A:75:ARG:CB	1:C:174:MET:HE2	2.43	0.49
1:A:246:ALA:HA	1:A:276:ALA:HA	1.94	0.49
1:A:265:LYS:HG3	1:B:302:VAL:CG1	2.43	0.49
1:A:226:ALA:N	1:A:227:PRO:CD	2.75	0.49
1:C:234:GLU:O	1:C:235:GLU:C	2.54	0.49
1:C:169:ALA:HB1	1:C:213:PHE:HZ	1.78	0.48
1:C:340:PRO:O	1:C:344:GLN:HG3	2.13	0.48
1:D:346:ILE:O	1:D:349:THR:HB	2.13	0.48
1:B:388:MET:HG3	1:D:82:PHE:HA	1.96	0.48
1:D:268:PHE:CD2	1:D:296:ILE:HD13	2.48	0.48
1:B:232:TRP:CD1	1:B:232:TRP:C	2.92	0.48
1:A:1:MET:HE2	2:A:448:HOH:O	2.13	0.47
1:B:36:GLY:HA3	1:B:104:ILE:HG13	1.96	0.47
1:A:38:GLY:HA3	1:A:96:GLY:O	2.15	0.47
1:B:124:ARG:HD3	2:B:435:HOH:O	2.13	0.47
1:B:167:ASP:HB2	1:B:208:GLY:O	2.14	0.47
1:C:357:ILE:HD12	1:C:357:ILE:N	2.30	0.47
1:D:134:LEU:HB2	1:D:137:HIS:CE1	2.49	0.47
1:D:172:TYR:HD2	1:D:388:MET:HE3	1.80	0.47
1:D:265:LYS:HG2	1:D:292:GLU:OE2	2.15	0.47
1:B:20:GLY:HA3	1:B:385:HIS:CE1	2.49	0.47
1:C:298:ALA:O	1:C:301:GLU:HB2	2.15	0.47
1:B:226:ALA:HB3	1:B:227:PRO:HD3	1.96	0.46
1:C:167:ASP:OD2	1:C:210:HIS:ND1	2.41	0.46
1:D:9:ILE:HD11	1:D:375:ARG:NH1	2.30	0.46
1:A:282:PRO:HB3	1:A:287:VAL:HG11	1.96	0.46
1:A:86:PRO:HB3	1:A:263:THR:HG23	1.98	0.46
1:B:248:VAL:O	1:B:252:VAL:HG22	2.16	0.46
1:C:222:GLY:HA3	1:C:252:VAL:HG11	1.98	0.46
1:C:229:SER:N	1:C:230:PRO:HD3	2.32	0.45
1:C:30:THR:HG23	1:C:104:ILE:HD13	1.98	0.45
1:C:95:SER:HB3	1:C:284:LEU:O	2.15	0.45
1:D:237:ILE:HB	1:D:238:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:GLU:O	1:D:235:GLU:C	2.59	0.45
1:B:43:ALA:O	1:D:81:GLY:HA3	2.16	0.45
1:B:81:GLY:HA3	1:D:43:ALA:O	2.17	0.45
1:A:37:TRP:CG	1:A:369:VAL:HG21	2.52	0.45
1:A:39:GLU:OE2	1:A:313:ALA:HB1	2.17	0.45
1:A:98:GLU:O	1:A:101:CYS:HB2	2.17	0.45
1:A:169:ALA:HB1	1:A:213:PHE:HZ	1.82	0.45
1:B:31:ASP:OD1	1:B:32:THR:HG23	2.16	0.45
1:A:75:ARG:HB3	1:C:174:MET:HE2	1.98	0.45
1:A:230:PRO:HG2	1:A:254:ILE:HG12	1.98	0.45
1:C:284:LEU:HD13	1:C:321:ASN:OD1	2.17	0.45
1:A:376:ALA:O	1:A:378:PRO:HD3	2.17	0.45
1:D:169:ALA:HB1	1:D:213:PHE:CZ	2.51	0.45
1:A:121:MET:HE1	1:D:174:MET:HE3	1.98	0.44
1:B:154:LEU:HD12	1:B:154:LEU:HA	1.82	0.44
1:A:180:PRO:HB3	1:A:213:PHE:CE1	2.53	0.44
1:C:226:ALA:N	1:C:227:PRO:CD	2.81	0.44
1:B:371:GLU:O	1:B:375:ARG:HG3	2.18	0.44
1:C:13:PRO:HA	1:C:14:PRO:HD3	1.90	0.44
1:D:172:TYR:CD2	1:D:388:MET:HE3	2.53	0.44
1:D:174:MET:O	1:D:174:MET:HG2	2.16	0.44
1:A:154:LEU:HD12	1:A:154:LEU:HA	1.87	0.44
1:A:234:GLU:O	1:A:235:GLU:C	2.60	0.44
1:B:174:MET:HG2	1:B:174:MET:O	2.18	0.44
1:C:106:GLY:HA3	1:C:364:GLY:HA2	1.99	0.44
1:A:204:ASP:OD1	1:D:182:MET:HG2	2.18	0.43
1:B:226:ALA:N	1:B:227:PRO:CD	2.82	0.43
1:D:130:TYR:CE1	1:D:165:LYS:HE3	2.53	0.43
1:B:172:TYR:HB3	1:B:212:GLN:HG3	1.99	0.43
1:C:232:TRP:C	1:C:232:TRP:CD1	2.96	0.43
1:C:318:TRP:CZ2	1:C:322:ILE:HD11	2.53	0.43
1:C:218:ALA:HB1	1:C:236:PRO:HB2	1.99	0.43
1:D:263:THR:HA	1:D:287:VAL:HA	2.00	0.43
1:B:49:ALA:O	1:B:53:VAL:HG23	2.18	0.43
1:A:36:GLY:HA3	1:A:104:ILE:HG13	2.00	0.43
1:B:98:GLU:OE1	1:B:289:GLY:HA3	2.19	0.43
1:B:246:ALA:HA	1:B:276:ALA:HA	2.01	0.43
1:D:174:MET:HE2	1:D:175:ARG:HG3	2.01	0.43
1:D:226:ALA:N	1:D:227:PRO:CD	2.82	0.43
1:A:66:ASN:HA	1:A:67:PRO:HD2	1.91	0.43
1:C:231:LEU:HD23	1:C:231:LEU:C	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:ARG:CB	1:D:174:MET:HE3	2.50	0.42
1:B:229:SER:N	1:B:230:PRO:CD	2.83	0.42
1:A:255:PRO:HB3	1:D:216:ALA:HB1	2.01	0.42
1:B:222:GLY:HA3	1:B:252:VAL:HG11	2.02	0.42
1:D:174:MET:HE1	1:D:175:ARG:HG3	2.00	0.42
1:B:13:PRO:HA	1:B:14:PRO:HD3	1.89	0.42
1:A:105:LEU:O	1:A:109:ARG:HG2	2.19	0.42
1:C:95:SER:HB2	1:C:285:GLY:O	2.20	0.42
1:B:85:ARG:HD2	1:D:88:LEU:HD22	2.01	0.42
2:A:443:HOH:O	1:D:179:MET:HE2	2.19	0.42
1:B:75:ARG:HB3	1:D:174:MET:HE3	2.02	0.42
1:B:344:GLN:HG3	1:B:373:LEU:HD21	2.01	0.42
1:C:328:ILE:HA	1:C:329:PRO:HD3	1.90	0.42
1:B:19:GLY:O	1:B:385:HIS:HE1	2.03	0.41
1:B:234:GLU:O	1:B:235:GLU:C	2.63	0.41
1:D:346:ILE:HD12	1:D:349:THR:HG22	2.02	0.41
1:C:27:LYS:HD2	1:C:37:TRP:CZ2	2.55	0.41
1:D:231:LEU:HD23	1:D:231:LEU:O	2.20	0.41
1:A:265:LYS:HB2	1:A:299:MET:HE1	2.01	0.41
1:C:20:GLY:HA3	1:C:385:HIS:CE1	2.54	0.41
1:C:128:TYR:HD1	1:C:333:MET:HG3	1.85	0.41
1:D:226:ALA:HB3	1:D:227:PRO:HD3	2.01	0.41
1:C:128:TYR:CD2	1:C:128:TYR:C	2.98	0.41
1:A:82:PHE:HA	1:C:388:MET:HG3	2.03	0.41
1:A:265:LYS:HG3	1:B:302:VAL:HG12	2.03	0.41
1:B:267:GLU:O	1:B:270:PRO:HD2	2.21	0.41
1:C:128:TYR:CD1	1:C:333:MET:HG3	2.55	0.41
1:B:348:SER:HB3	1:B:351:LYS:HD2	2.02	0.41
1:D:36:GLY:HA3	1:D:104:ILE:HG13	2.02	0.41
1:D:172:TYR:HB3	1:D:212:GLN:HG3	2.03	0.41
1:C:36:GLY:HA3	1:C:104:ILE:HG13	2.02	0.41
1:D:117:ILE:HD12	1:D:294:LYS:HD3	2.02	0.41
1:A:121:MET:HE1	1:D:174:MET:CE	2.51	0.41
1:C:68:GLU:HG2	1:C:109:ARG:NH2	2.35	0.41
1:B:39:GLU:OE2	1:B:313:ALA:HB1	2.21	0.41
1:C:4:GLN:HG2	1:C:5:ASP:CG	2.45	0.41
1:B:139:MET:HE2	1:B:139:MET:HB3	1.87	0.40
1:B:268:PHE:CD2	1:B:296:ILE:HD13	2.56	0.40
1:A:72:LEU:HD12	1:C:174:MET:HE1	2.04	0.40
1:C:169:ALA:HB1	1:C:213:PHE:CZ	2.54	0.40
1:C:299:MET:O	1:C:302:VAL:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:ILE:HD11	1:B:375:ARG:NH1	2.37	0.40
1:D:21:ARG:HD3	2:D:462:HOH:O	2.20	0.40
1:D:272:LEU:HD21	1:D:280:LEU:HD11	2.03	0.40
1:A:174:MET:HE3	1:A:174:MET:HB3	1.87	0.40
1:D:284:LEU:HD11	1:D:324:LEU:HD22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	394/432 (91%)	372 (94%)	22 (6%)	0	100	100
1	B	394/432 (91%)	371 (94%)	22 (6%)	1 (0%)	36	53
1	C	394/432 (91%)	378 (96%)	16 (4%)	0	100	100
1	D	394/432 (91%)	374 (95%)	20 (5%)	0	100	100
All	All	1576/1728 (91%)	1495 (95%)	80 (5%)	1 (0%)	48	67

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1	MET

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	303/332 (91%)	288 (95%)	15 (5%)	22	42
1	B	303/332 (91%)	291 (96%)	12 (4%)	28	51
1	C	303/332 (91%)	295 (97%)	8 (3%)	40	66
1	D	303/332 (91%)	292 (96%)	11 (4%)	31	55
All	All	1212/1328 (91%)	1166 (96%)	46 (4%)	29	53

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	6	LEU
1	A	85	ARG
1	A	89	THR
1	A	91	MET
1	A	154	LEU
1	A	173	THR
1	A	174	MET
1	A	202	LYS
1	A	209	THR
1	A	232	TRP
1	A	243	GLU
1	A	265	LYS
1	A	287	VAL
1	A	361	THR
1	B	25	LEU
1	B	85	ARG
1	B	120	ARG
1	B	154	LEU
1	B	164	ILE
1	B	173	THR
1	B	174	MET
1	B	209	THR
1	B	258	THR
1	B	264	THR
1	B	324	LEU
1	B	380	THR
1	C	85	ARG
1	C	164	ILE
1	C	173	THR
1	C	209	THR
1	C	243	GLU
1	C	307	ILE

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Mol	Chain	Res	Type
1	C	343	ASP
1	C	357	ILE
1	D	85	ARG
1	D	89	THR
1	D	130	TYR
1	D	164	ILE
1	D	174	MET
1	D	209	THR
1	D	232	TRP
1	D	242	VAL
1	D	264	THR
1	D	338	GLU
1	D	349	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	306	GLN
1	B	136	HIS
1	B	223	ASN
1	B	385	HIS
1	C	310	HIS
1	C	344	GLN
1	D	136	HIS
1	D	210	HIS
1	D	310	HIS
1	D	385	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	396/432 (91%)	-0.36	1 (0%) 90 88	10, 16, 25, 43	0
1	B	396/432 (91%)	-0.33	1 (0%) 90 88	10, 16, 29, 42	0
1	C	396/432 (91%)	-0.33	0 100 100	10, 17, 29, 41	0
1	D	396/432 (91%)	-0.39	1 (0%) 90 88	11, 16, 27, 47	0
All	All	1584/1728 (91%)	-0.35	3 (0%) 91 90	10, 16, 28, 47	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	139	MET	2.7
1	B	0	SER	2.4
1	D	130	TYR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.